

Cyclophosphamide  
50-18-0 | DTXSID5020364

Model Performance

Model

Data

Weighted KNN model

| 5-fold CV (75%) |      | Training (75%) |      | Test (25%) |      |
|-----------------|------|----------------|------|------------|------|
| Q2              | RMSE | R2             | RMSE | R2         | RMSE |
| 0.91            | 1.08 | 0.91           | 1.08 | 0.92       | 1.00 |

Model Results

Predicted value: 9.81e-05 mmHg

Global applicability domain: Inside

Local applicability domain index: 4.37e-01

Confidence level: 3.26e-01

Nearest Neighbors from the Training Set

|  |  |  |
|--|--|--|
| <div>Image not found</div> <div>Piperophos</div> <div>Measured: 5.48e-02</div> <div>Predicted: 3.95e-07</div>                    | <div>Image not found</div> <div>Benazolin-ethyl</div> <div>Measured: 2.89e-07</div> <div>Predicted: 9.58e-07</div> | <div>Image not found</div> <div>Isoproturon</div> <div>Measured: 7.95e-05</div> <div>Predicted: 6.19e-08</div> |
| <div>Image not found</div> <div>Tris(2-chloroethyl) phosphate</div> <div>Measured: 3.47e-05</div> <div>Predicted: 2.39e-02</div> |  |  |